

# Inhomogeneous Cooling of the Rough Granular Gas in Two Dimensions

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**Abstract** – We study the inhomogeneous clustered regime of a freely cooling granular gas of rough particles in two dimensions using large-scale event driven simulations and scaling arguments. During collisions, rough particles dissipate energy in both the normal and tangential directions of collision. In the inhomogeneous regime, translational kinetic energy and the rotational energy decay with time  $t$  as power-laws  $t^{-\theta_T}$  and  $t^{-\theta_R}$ . We numerically determine  $\theta_T \approx 1$  and  $\theta_R \approx 1.6$ , independent of the coefficients of restitution. The inhomogeneous regime of the granular gas has been argued to be describable by the ballistic aggregation problem, where particles coalesce on contact. Using scaling arguments, we predict  $\theta_T = 1$  and  $\theta_R = 1$  for ballistic aggregation,  $\theta_R$  being different from that obtained for the rough granular gas. Simulations of ballistic aggregation with rotational degrees of freedom are consistent with these exponents.

**Introduction.** – The freely cooling granular gas is a collection of ballistic particles that undergo momentum conserving inelastic collisions in the absence of any external driving. It is the simplest system to study large scale effects of inelasticity and has found application in varied physical phenomena including modelling of dynamics of granular systems [1–5], geophysical flows [6], large-scale structure formation in the universe [7], and shock propagation [8–10]. It also belongs to the general class of non-equilibrium systems with limiting cases being amenable to exact analysis [11, 12], and is an example of an ordering system showing non-trivial coarsening behavior [13–16]. The dynamics of this system has close connection with the shock dynamics of the well studied Burgers equation [11, 17–20]. Of primary interest is the temporal evolution of the translational kinetic energy  $T(t)$  and rotational energy  $R(t)$  at large times.

Realistic models of non-sliding collisions of hard spheres involve two parameters: (a) the coefficient of normal restitution  $r$ , quantifying the dissipation in the normal direction of collision, and (b) the coefficient of tangential restitution  $\beta$ , quantifying the dissipation in tangential direction for collisions [21–25]. In most studies of the freely cooling granular gas, the parameter  $\beta$  characterizing tangential dissipation is ignored, and this simplified model is referred to as the smooth granular gas (SGG). The rota-

tional energy of SGG is conserved, but the translational kinetic energy decreases with time.

At initial times of the evolution of SGG, particles remain homogeneously distributed and  $T(t)$  decreases with time  $t$  as  $t^{-2}$  (Haff’s law) [26–30]. At later times, this regime is destabilized by long wavelength fluctuations into an inhomogeneous regime dominated by clustering of particles [31–33]. In this inhomogeneous regime,  $T(t)$  decreases as a power law  $t^{-\theta_T}$ , where  $\theta_T \neq 2$  depends only on the dimension  $d$ . Extensive simulations in one [34], two [35] and three [36] dimensions show that, for large times and  $r < 1$ , the system resembles a sticky gas ( $r \rightarrow 0$ ) such that colliding particles effectively coalesce and form aggregates, thus resembling the well studied ballistic aggregation model (BA). A scaling analysis of BA for spherical aggregates in the dilute limit predicts  $\theta_T = 2d/(d+2)$  [37]. Simulations of SGG in one, two and three dimensions are in excellent agreement with this result [34–36]. Surprisingly,  $\theta_T$  for BA depends on the density and converges to the above expression only in the dense limit [36, 38, 39]. Since the derivation in Ref. [37] assumes the dilute limit and ignores velocity correlations, it has been argued that the energy decay in the SGG being described accurately by  $\theta_T = 2d/(d+2)$  is a coincidence [36, 38, 39].

When the collisions include tangential dissipation  $\beta$ , the translational and rotational modes are no longer indepen-

dent of each other [40–48]. We call this model the rough granular gas (RGG). Studies of RGG have been limited to the homogeneous regime. In this regime, kinetic theory [40–45] and simulations [44, 45] show that both translational energy  $T(t)$  and rotational energy  $R(t)$  decreases at  $t^{-2}$ . However, the partitioning of energy into the rotational and translational modes does not follow equilibrium equipartitioning, and depends on both  $r$  and  $\beta$ . In addition, the directions of the translational and angular velocities of a particle were found to be strongly correlated [46, 49].

The inhomogeneous clustered regime of RGG is poorly studied. In this paper, we study the inhomogeneous regime of two dimensional RGG using large scale event driven molecular dynamics simulations. Let  $T(t) \sim t^{-\theta_T}$  and  $R(t) \sim t^{-\theta_R}$  in this regime. We show that  $\theta_T$  is independent of  $\beta$  and is the same as that for SGG, i.e.,  $\theta_T \approx 1$ . The exponent  $\theta_R$  is also shown to be independent of the choice of  $r$  and  $\beta$ ,  $|\beta| < 1$  and to be  $\theta_R = 1.60 \pm 0.04$ , different from  $\theta_R = 2$  in the homogeneous regime. Thus, unlike the homogeneous regime, the two exponents  $\theta_T$ ,  $\theta_R$  differ from each other. These exponents are compared with the corresponding exponents for BA with rotational degree of freedom. The translational energy of BA is independent of its rotational degrees of freedom and hence  $\theta_T \approx 1$  for large enough initial densities [39]. Numerically, we find that  $\theta_R \approx 1$  for BA. We conclude that the large time limit of RGG is different from that of BA, even though clustering is present. Finally, we extend the scaling arguments of Ref. [37] to BA with rotational degree of freedom. The scaling arguments predict  $\theta_R = 1$  in two dimensions. This is clearly in contradiction with the numerically obtained value of  $1.6 \pm 0.04$ . This further supports the view [36, 38, 39] that the energy decay in the SGG being described accurately by  $\theta_T = 2d/(d+2)$  is a coincidence.

**Model and Collision Laws.** – Consider a system of  $N$  hard disks confined in a two-dimensional volume of linear length  $L$  with periodic boundary conditions in both directions. To each particle  $i$  located at  $\vec{r}_i$ , we associate a velocity  $\vec{v}_i$ , an angular velocity  $\vec{\omega}_i$ , a mass  $m_i$  and a radius  $a_i$ . The moment of inertia is given by  $I_i = qm_i a_i^2$ , where  $q = 1/2$  for a disk. A particle moves ballistically till it collides with another particle.

We first define the collision law in the RGG model. All particles are considered identical, i.e.,  $m_i = m$  and  $a_i = a$  for all  $i$ . Consider a collision between two particles  $i$  and  $j$ , moving with velocities  $\vec{v}_i$ ,  $\vec{v}_j$  and angular velocities  $\vec{\omega}_i$ ,  $\vec{\omega}_j$ . The relative velocity  $\vec{g}_{ij}$ , between  $i$  and  $j$  of the point of contact is

$$\vec{g}_{ij} = (\vec{v}_i - \vec{\omega}_i \times a\vec{e}) - (\vec{v}_j + \vec{\omega}_j \times a\vec{e}), \quad (1)$$

where  $\vec{e}$  is the unit vector pointing from the center of particle  $j$  to center of particle  $i$ . We denote the normal and tangential components of  $\vec{g}_{ij}$  by  $\vec{g}_{ij}^n$  and  $\vec{g}_{ij}^t$  respectively. The dissipation in normal and tangential directions is quanti-

fied by a coefficient of normal restitution  $r$  and a coefficient of tangential restitution  $\beta$ , defined through the constitutive equations [50]:

$$(\vec{g}_{ij}^n)' = -r\vec{g}_{ij}^n, \quad 0 \leq r \leq 1, \quad (2)$$

$$(\vec{g}_{ij}^t)' = -\beta\vec{g}_{ij}^t, \quad -1 \leq \beta \leq 1, \quad (3)$$

where the primed symbols denote the post-collision values. Equations (2) and (3), combined with linear and angular momentum conservation for hard spheres, yield the post-collision velocities as

$$\vec{v}'_{i,j} = \vec{v}_{i,j} \mp \frac{1+r}{2}\vec{g}_{ij}^n \mp \frac{q(\beta+1)}{2(q+1)}\vec{g}_{ij}^t, \quad (4)$$

$$\vec{\omega}'_{i,j} = \vec{\omega}_{i,j} + \frac{\beta+1}{2a(q+1)}(\vec{e} \times \vec{g}_{ij}^t). \quad (5)$$

Translational kinetic energy and rotational energy are both conserved only when  $r = 1$  (elastic) and  $\beta = -1$ . In this paper, we assume  $r$  and  $\beta$  to be constant, independent of the relative velocity of collision.

In the BA model, particles move ballistically and on collision merge to become a new particle, whose shape is assumed to be spherical. Consider the collision between particles  $i$  and  $j$ . The mass  $m'$  of the new particle is given by mass conservation

$$m' = m_i + m_j, \quad (6)$$

and its velocity  $\vec{v}'$  is given by linear momentum conservation

$$m'\vec{v}' = m_i\vec{v}_i + m_j\vec{v}_j. \quad (7)$$

The radius  $a'$  of the new particle is obtained from volume conservation:  $a'^2 = a_i^2 + a_j^2$ . The position  $\vec{r}'$  of the new particle is obtained from the conservation of center of mass:

$$m'\vec{r}' = m_i\vec{r}_i + m_j\vec{r}_j. \quad (8)$$

The new angular velocity  $\vec{\omega}'$  is obtained from conservation of angular momentum. Let  $I' = qm'a'^2$  be the moment of inertia of the new particle. Then,

$$I'\vec{\omega}' = I_i\vec{\omega}_i + I_j\vec{\omega}_j + \frac{m_i m_j}{m_i + m_j}(\vec{r}_i - \vec{r}_j) \times (\vec{v}_i - \vec{v}_j). \quad (9)$$

Equations (6)–(9) completely determine the mass, position, velocity and angular velocity of the new particle.

The quantities of interest in this paper are the translational and rotational energy defined as

$$T(t) = \frac{1}{K} \sum_{i=1}^{S(t)} \frac{1}{2} m_i v_i^2(t), \quad (10)$$

$$R(t) = \frac{1}{K} \sum_{i=1}^{S(t)} \frac{1}{2} I_i \omega_i^2(t), \quad (11)$$

where these energies are scaled by the initial translational energy  $K = T(0)$  and  $S(t)$  is the total number of particles

in the system at time  $t$ . For RGG,  $S(t) = N$ , while for BA it decreases with time.

We simulate both RGG and BA in two dimensions using event driven molecular dynamics simulations [51]. Inelastic collapse [52, 53] is avoided by making collisions elastic when the relative velocity of the colliding particles is less than a cutoff  $\delta$  [34]. This cutoff velocity introduces a timescale beyond which collisions are mostly elastic, and the systems crosses over to a new regime where energy is a constant. In our simulations, we choose  $\delta = 10^{-5}$  for which we check that this crossover timescale is much larger than the largest time in our simulations. Thus, the results presented in the paper are independent of  $\delta$ .

The initial mass and diameter of the disks are taken to be unity. The particles are initially uniformly distributed, and the translational and angular velocities are drawn from a Gaussian distribution with mean zero and variance 1 and 8 respectively. The variances are such that  $T(0) = 2R(0)$ . Thus, energy is equipartitioned between all three modes as one would expect in equilibrium. The results in this paper are for systems of  $N = 1562500$  particles and  $L = 2500$  (volume fraction = 0.20).

**Scaling theory for rotational energy in ballistic aggregation.** – The exponent  $\theta_R$  for BA may be determined using scaling arguments. In BA, particles form spherical aggregates on collision. We first recapitulate the calculation of  $\theta_T = 2d/(d+2)$  [37] as outlined in Refs. [38, 54]. Let  $n$  be the number density. It evolves in time as

$$\frac{dn}{dt} = -\frac{n}{\tau}, \quad (12)$$

where  $\tau$  is the mean collision time. In  $d$  dimensions,

$$\frac{1}{\tau} \sim nv_{rms}R_t^{d-1}, \quad (13)$$

where  $v_{rms}$  is the root mean squared velocity and  $R_t$  is the radius of a typical aggregate at time  $t$ . Since total mass is conserved,  $M_t n \sim 1$  or equivalently  $R_t \sim n^{-1/d}$ . Substituting for  $\tau$  from Eq. (13) in Eq. (12),

$$\frac{dn}{dt} \sim -n^{1+1/d}v_{rms}. \quad (14)$$

The dependence of  $v_{rms}$  on  $M_t$  is required. An aggregate of mass  $M_t$  is formed by aggregation of  $M_t$  particles of mass 1. Conservation of linear momentum, combined with the assumption of uncorrelated momenta, gives  $M_t v_{rms} \sim M_t^{1/2}$ , or  $v_{rms} \sim n^{1/2}$ . Substituting for  $v_{rms}$  in Eq. (14), we obtain

$$n(t) \sim t^{-2d/(d+2)}. \quad (15)$$

The scaling of root mean square angular velocity  $\omega_{rms}$  with time  $t$  may be obtained from conservation of angular momentum. If two particles  $i$  and  $j$  of masses  $m_i, m_j$  at  $\vec{r}_i, \vec{r}_j$ , moving with velocities  $\vec{v}_i, \vec{v}_j$ , angular velocities  $\vec{\omega}_i, \vec{\omega}_j$ , and moment of inertia  $I_i$  and  $I_j$  collide to form a

particle of mass  $m'$  at  $\vec{r}'$  with velocity  $\vec{v}'$ , and moment of inertia  $I'$ , then its angular velocity  $\vec{\omega}'$  is given by Eq. (9).

Let  $\omega_{rms}$  be the root mean square angular velocity of the typical particle whose moment of inertia is  $I_t \sim M_t R_t^2$ . In Eq. (9), there are three terms on the right hand side. We first assume that the right hand side is dominated by the first two terms. Then the angular momentum  $I_t \omega_{rms}$  is a sum of  $M_t$  random variables of mean zero and variance order 1, giving

$$I_t \omega_{rms} \sim \sqrt{M_t}. \quad (16)$$

or equivalently  $\omega_{rms} \sim M_t^{-(d+4)/(2d)}$ . But the rotational energy  $R(t)$  scales as  $R \sim n I_t \omega_{rms}^2$ . Simplifying, we obtain  $R \sim t^{-2}$ , independent of dimension. We now assume that the right hand side of Eq. (9) is dominated by the third term. Then, clearly  $I_t \omega_{rms} \sim M_t R_t v_{rms}$ . Using  $M_t n \sim 1$ , we obtain  $\omega_{rms} \sim n^{(d+2)/(2d)} \sim t^{-1}$ . The rotational energy  $I_t \omega_{rms}^2$  now scales as  $t^{-2d/(d+2)}$ . This has a slower decay in time than  $t^{-2}$  obtained from assuming that Eq. (9) is dominated by the first two terms. The kinetic energy  $T \sim n M_t v_{rms}^2$  and rotational energy  $R$  are thus given by

$$T \sim t^{-2d/(d+2)}, \quad (17)$$

$$R \sim t^{-2d/(d+2)}, \quad (18)$$

implying that  $\theta_T = \theta_R = 2d/(d+2)$ . Thus, one expects that the ratio of the two energies is a constant in the clustered inhomogeneous regime as it is in the homogeneous regime.

### Simulation Results. –

*Rough granular gas (RGG).* We now present results for RGG obtained from numerical simulations. Figure 1 shows the temporal evolution of translational kinetic energy  $T(t)$ . Here, the coefficient of normal restitution  $r = 0.1$ . For this value of  $r$ , the homogeneous regime is short lived. The crossover time from the homogeneous to inhomogeneous regime depends on  $\beta$ , the crossover time increasing with  $|\beta|$ . This is expected as increasing  $|\beta|$  correspond to decreasing dissipation, and hence a longer homogeneous regime. For  $\beta < 0$ , the dependence of the crossover time on  $\beta$  is very weak. For all values of  $\beta$ , the data is consistent with  $\theta_T = 1$  (see Fig. 1), same as that obtained for SGG [35]. We check that the  $\theta_T$  remains the same for  $r = 0.5$  and  $r = 1.0$  (but  $|\beta| < 1$ ). We conclude that  $\theta_T$  for RGG is independent of the values of both  $r$  and  $\beta$ . These extend the results obtained earlier for SGG ( $\beta = -1$ ), where  $\theta_T$  was shown to be independent of  $r$  [34–36].

Figures 2 and 3 show the temporal evolution of rotational energy  $R(t)$  for  $\beta > 0$  and  $\beta < 0$  respectively. The crossover to inhomogeneous regime occurs at a much later time when compared with  $T(t)$ . A signature of this difference in crossover times was observed in Ref. [45], where  $T$  was found to deviate from the homogeneous cooling behavior of  $t^{-2}$  decay, while  $R$  still followed it. We also observe

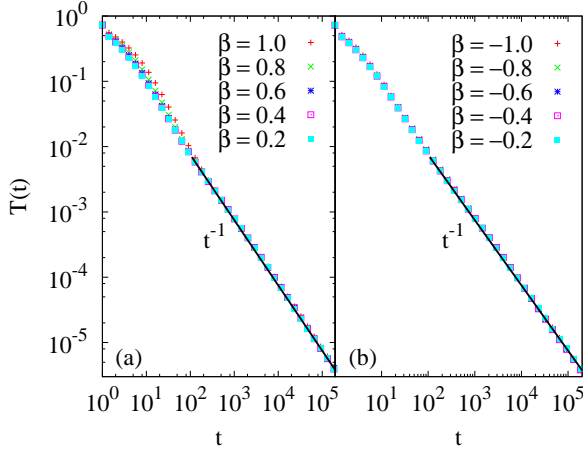


Fig. 1: (Color online) Time evolution of translational kinetic energy  $T(t)$  for RGG when (a)  $\beta > 0$  and (b)  $\beta < 0$  for fixed  $r = 0.10$ .

that the crossover times are much larger for  $\beta < 0$  as compared to that  $\beta > 0$ . When  $\beta = -1$ ,  $R(t)$  is conserved. At large times, the data for  $R(t)$  are completely independent of  $\beta$  (see Figs. 2 and 3). We estimate  $\theta_R = 1.60 \pm 0.04$ .

We also confirm that  $\theta_R$  is independent of  $r$ . In Fig. 4, we show the dependence of  $R(t)$  on  $r$  by varying  $r$  and keeping  $\beta = 0.60$  fixed.  $R(t)$ , while decaying with a  $r$ -independent exponent, now has a  $r$ -dependent pre-factor. Thus, we conclude that at large times,  $R(t) \simeq A(r)t^{-\theta_R}$ , where  $\theta_R \approx 1.60$  is independent of  $r$  and  $\beta$ .

**Ballistic aggregation (BA).** We now present the results from numerical simulations of BA. In these simulations, whenever two particles collide we replace them with a single spherical particle conserving mass, volume, linear and angular momenta as described in Eqs. (6)–(9). If the new particle overlaps with another particle, then these two particles aggregate. Thus, a collision between two particles may give rise to a chain of aggregation events.

For BA, it is easy to check from Eqs. (6) and (7) that including rotational degrees of freedom does not affect the translational kinetic energy  $T(t)$ . That being the case, we expect that  $\theta_T$  for the rough BA to be identical to that for the smooth BA. The numerical values of  $\theta_T$  for the rough BA for different initial volume fraction  $\phi$  are tabulated in the second column of Table 1.  $\theta_T$  depends weakly on  $\phi$  [36, 38, 39], and approaches 1 with increasing  $\phi$ .  $\theta_T = 1$  for BA is consistent with the scaling arguments [see Eq. (18)], and is equal to  $\theta_T$  for RGG.

The variation of the rotational kinetic energy  $R(t)$  for BA with time  $t$  is shown in Fig. 5. Similar to  $\theta_T$ ,  $\theta_R$  also decreases with increasing volume fraction  $\phi$  (see third column of Table 1). With increasing  $\phi$ ,  $\theta_R$  converges to a value very close to 1, different from that obtained for RGG. Note that the scaling argument for BA predicts  $\theta_R = 1$  (see Eq. 18).

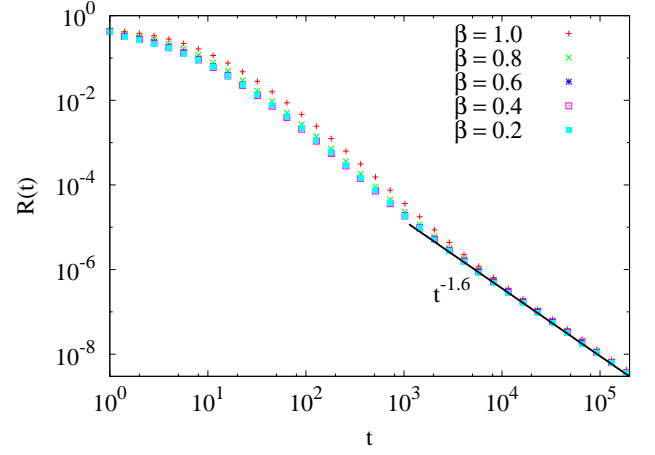


Fig. 2: (Color online) Time evolution of rotational energy  $R(t)$  of RGG for  $\beta > 0$  and fixed  $r = 0.10$ .

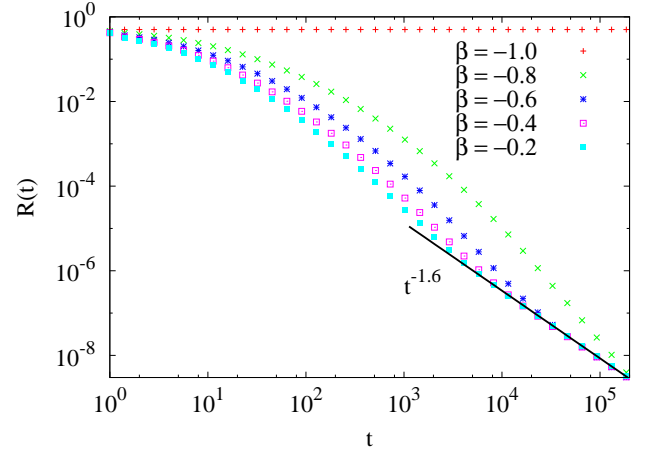


Fig. 3: (Color online) Time evolution of rotational energy  $R(t)$  of RGG for  $\beta < 0$  and fixed  $r = 0.10$  in RGG.

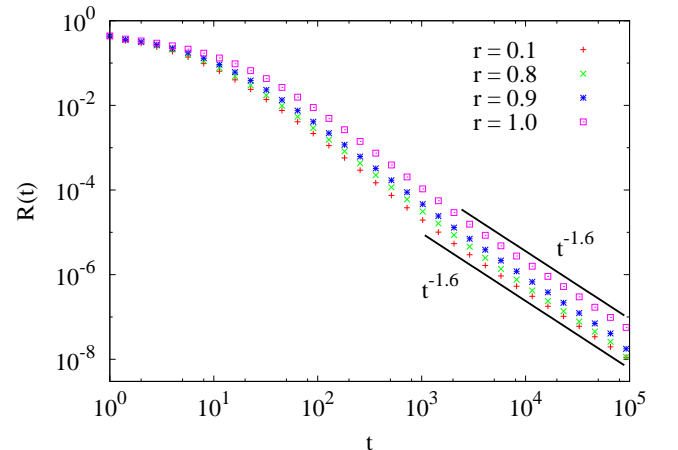


Fig. 4: (Color online) Time evolution of rotational energy  $R(t)$  of RGG for different  $r$  and fixed  $\beta = 0.60$ .

Table 1: Dependence of exponents  $\theta_T$  and  $\theta_R$  on volume fraction  $\phi$  in the BA model.

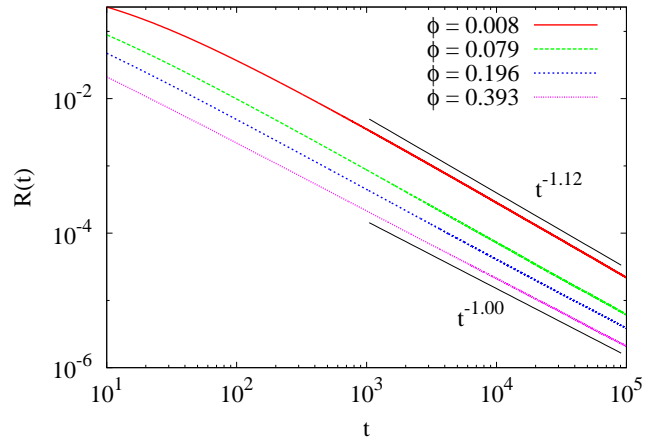
$\phi$	$\theta_T$	$\theta_R$
0.008	1.12-1.13	1.10-1.12
0.079	1.05-1.06	1.07-1.08
0.196	1.01-1.02	1.03-1.04
0.393	1.01-1.02	1.00-1.01

**Conclusion and discussion.** — To summarize, we investigated the large time behavior of a freely cooling rough granular gas in two dimensions using event-driven simulations. Each collision dissipates energy in both the normal and tangential directions. We showed that in the clustered inhomogeneous regime, both the translational kinetic energy  $T(t)$  and the rotational energy  $R(t)$  decay with time  $t$  as power-laws  $A_T t^{-\theta_T}$  and  $A_R t^{-\theta_R}$  where  $\theta_T \approx 1.0$ , and  $\theta_R \approx 1.6$ . These exponents are universal and independent of  $r$  and  $\beta$ . Within numerical errors,  $A_T$  is also independent of  $r$  and  $\beta$ , while  $A_R$  depends only on  $r$ . For ballistic aggregation with rotational degree of freedom, wherein particles coalesce on contact, we find that  $\theta_T \approx 1.0$  and  $\theta_R \approx 1.0$  for large enough initial volume fraction  $\phi$ . By extending an earlier scaling theory for BA, we obtain  $\theta_R = 1$ , consistent with the numerically obtained value.

Kinetic theory for granular gases predicts that  $R(t)/T(t)$  tends to a non-zero constant that depends on  $r$  and  $\beta$  [43–45]. In the inhomogeneous regime, since  $\theta_T < \theta_R$  for the rough granular gas, the ratio  $R(t)/T(t)$  tends to zero at large times. Violation of kinetic theory is not surprising given that it assumes that particles are homogeneously distributed, which is not the case in the inhomogeneous regime.

It has been earlier shown that in the homogeneous regime, the directions of the angular velocity and translational velocity are correlated [46]. It would be interesting to see whether this holds true in the inhomogeneous regime in three dimensions. Unfortunately, simulations in three dimensions have strong finite size effects [36] and at the same time the crossover time from the homogeneous regime to inhomogeneous regime for the rotational energy is large. This makes it difficult to obtain a large enough temporal regime where one may test for correlation. This is a promising area for future study.

The clustered regime of the freely cooling granular gas has been often thought to be describable by the large time behavior of the ballistic aggregation model. This analogy has been reinforced in particular by the fact that, within numerical error, energy decay in both systems is the same in one, two and three dimensions [34–36]. However, it has been shown that correlation functions that capture spatial distribution of particles and the velocity distributions in the granular gas are different from that of BA [14, 36]. In particular, it has been argued that a coarse grained model


 Fig. 5: (Color online) Time evolution of the rotational energy  $R(t)$  of BA for different volume fractions  $\phi$ .

with aggregation and fragmentation is more suitable to study the clustered regime than one of pure aggregation as in the BA model [16]. Here, the fact that the rotational energies in the two models decay with two exponents is further evidence that the analogy should be used with care.

In the scaling arguments presented in this paper and in Ref. [37], the correlations between velocities of colliding particles are ignored. Therefore, it has often been argued that the efficacy of the scaling arguments is a coincidence [38, 39]. In this paper, we showed that the extension of the scaling arguments to rotational energies correctly predict the numerical results for BA, albeit for larger volume fractions  $\phi$ . We conclude that the scaling arguments are quite robust, rather the connection to granular gas is more suspect.

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The simulations were carried out on the supercomputing machine Annapurna at The Institute of Mathematical Sciences.

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